**iMetaLab 1.0: A web platform for metaproteomics data analysis**

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**Supplementary Data**

S1 iMetaLab platform architecture

The iMetaLab platform is composed of servers that both host the MetaLab software and process client-side requests, and a front-end web interface that gathers client-side requests and displays corresponding server-side responses. The communication between the client and server is handled through stateless HTTP requests. The front-end web interface of iMetaLab is built using a javascript library, React.js, which allowed for creation of a single-page application (SPA) web application capable of generating highly interactive web interfaces without requiring page reloads. The servers of iMetaLab are configured in Apache that handle HTTP requests through an interface designed as RESTful APIs written in PHP language.

S2 iMetaLab sample run-through

In this supplementary data section, we describe a complete run-through of metaproteomic data analysis using iMetaLab’s web interface.

S2.1 Access iMetaLab web interface

The session parameters and the generated results are available on iMetaLab’s website. The web interface can be accessed through “http://imetalab.ca” by clicking the “Enter iMetaLab” button on the main page, or can be accessed directly through “http://dashboard.imetalab.ca”.

S2.2 Setup a new Session

iMetaLab server allows each submission up to 10 raw files with size of 3G for each. iMetaLab manages each session in a stateless manner meaning that the server does not track or maintain user’s status, but simply answers to requests based on valid session IDs. Therefore, when setting up a new session, once that session is authenticated, the server does not track any of the activities happening inside of the user’s web browser, such as at which step the user is or which of the parameters have been selected. When a user decides to submit the task to the server, by clicking “Submit”, the user sends a request to the server with the submitted data. For each submission, the server simply responds by accepting the submission and initiating MetaLab to perform data analysis. The same server-client communication channel is used for the progress tracking feature of iMetaLab.

A new session was initiated by navigating to “Create Session” tab under “Data processing” category. A new unique session ID was obtained by submitting a valid email address. The new session was created by logging into the session using the received session ID, uploading raw files, selecting database and updating corresponding parameters. The process was completed in four steps with the following order:

1. Enter the session ID for authentication.

2. Upload raw files.

3. Select a database (mouse database was selected for demonstration).

4. Modify all necessary parameters before the submission. This demonstration session used default settings for all the parameters.

The session was submitted to iMetaLab server by first clicking the “Preview” button followed by clicking the “Submit” button.

S2.3 Track the Session

The progress of the submitted session was tracked through the “View Results” tab under the “Data processing” category. After completion, the following files were generated and listed in result table: “MetaLab.iMetaLab.tree.csv”, “function.csv”, “msms.txt”, “peptides.txt”, “proteinGroups.txt”, “summary.txt”, “MetaLab.taxonomy.xlsx”, “Biom\_MetaLab.biom”.

All the files are available on iMetaLab’s website through a public available session ID, metasess\_5982077a2bf951.10052915.

The processing time varies based on whether the mouse or human microbiome database is selected. The total processing time for mouse microbiome database is approximately 30 hours for 10 raw files with the size of each up to 3G. For human microbiome database, the total processing time is approximately 70 hours.

S2.4 Visualize Data

To view MS performance, click “Bar Chart” to launch the visualization window. To view taxonomy profile, click either “Tree Chart” or “Pie Chart” to launch the corresponding visualization window.

S3 iMetaLab data visualization

The visualization tools of iMetaLab were developed using basic HTML5, CSS3 and JavaScript, with two supporting JavaScript based libraries: D3.js and jQuery. This design allows visualizations to be generated inside the browser rather than relying on a remote server to process the visualization data, which means use of the visualization tools are not restricted to iMetaLab generated files. Each visualization window is provided with an “Upload” button to read visualization ready files. As long as the submitted data structure matches the required format, visualization features will work for any data contents. Sample data are available on iMetaLab to provide users with examples on how to format their own data to use the visualization tools.